

Renormalization group method for weakly coupled quantum chains: comparison with exact diagonalization

J.V. Alvarez¹ and S. Moukouri^{1,2}

¹*Department of Physics, University of Michigan,*

²*Michigan Center for Theoretical Physics 2477 Randall Laboratory, Ann Arbor MI 48109*

(Dated: February 2, 2008)

We show that numerical quasi-one-dimensional renormalization group allows accurate study of weakly coupled chains with modest computational effort. We perform a systematic comparison with exact diagonalization results in two and three-leg spin ladders with a transverse Hamiltonian that can involve frustration. Due to the variational nature of the algorithm, the accuracy can be arbitrarily improved enlarging the basis of eigenstates of the density matrix defined in the transverse direction. We observe that the precision of the algorithm is directly correlated to the binding of the chains. We also show that the method performs especially well in frustrated systems.

I. INTRODUCTION

It was recently shown¹ that a general Kato-Bloch matrix expansion can be applied to weakly-coupled quantum chains. This algorithm was used to study weakly-coupled Heisenberg chains^{2,3}. The DMRG was used as the method of solution for an isolated chain and then again for the solution of an effective 1D model which is obtained by projecting the problem to the basis of the tensor product of independent chain states. A good agreement with the stochastic series expansion (SSE) quantum Monte Carlo (QMC) was found for transverse couplings J_{\perp} not too large. Then interchain diagonal exchange J_d which frustrates the system was introduced. It is found, by analyzing ground state energies and spin-spin correlation functions, that there is a transition between two ordered magnetic states. When $J_d/J_{\perp} \lesssim 0.5$, the ground state displays a Néel order. When $J_d/J_{\perp} \gtrsim 0.5$, a collinear magnetic ground state in which interchain spin correlations are ferromagnetic becomes stable. In the vicinity of the transition point, $J_d/J_{\perp} \approx 0.5$, the ground state is disordered. The prediction of a disordered ground state is of central importance for two reasons. First, because a recent neutron scattering experiment⁴ on the frustrated AFM Cs_2CuCl_4 has predicted a spin liquid ground state in this material. Second, a disordered doped spin liquid has been conjectured to be relevant for the physics of high temperature cuprate superconductors. The search of this disordered two-dimensional state by numerical methods has been challenging. Cluster QMC methods^{5,6}, that have been extremely useful in nonfrustrated spin systems, are hampered by sign problems for Hamiltonians with finite J_d , making very difficult their study by this technique. New algorithms have been specifically designed to deal with frustration and intense numerical research has been devoted to these systems^{7,8,9}. It is thus of central importance to show that the DMRG prediction is correct.

We address in this paper several questions that increase the understanding and show new potential of the method, giving additional support for the physical findings of Ref. 3. Some of these questions are technical

in nature and they demand exhaustive comparison with exact results.

The class of models that we study here have transverse terms involving competing interactions. These transverse terms are projected in a optimal reduced basis of eigenstates of the independent chain. If, for instance, the chains are coupled with perpendicular and diagonal exchange constants (see the left ladder in Fig. 1), the projection of the perpendicular (J_{\perp}) and the diagonal (J_d) parts of the interchain coupling is qualitatively different one to the other. More precisely, to represent coupling terms along the diagonal requires matrix elements of operators defined in different sites (those usually associated with the computation of short range correlation functions in 1D DMRG calculations). It is this competing behavior what generates negative local Boltzmann weights (sign problems) that can not be eliminated by canonical transformations when QMC is used. Therefore, it is important to check if all competing terms are represented and treated with similar accuracy by studying models that mix these terms in different ways.

We will also show that the accuracy is directly correlated to the binding energy of the chains and not to the nominal values of the transverse couplings, concluding that the method is specially good for the study of frustrated systems. In addition, based on the results of this study we have designed internal tests that signal good performance of the method when dealing with larger lattices where comparison with exact data is not possible.

Finally, we are also interested in showing the controllability of the approximation involved in the method, specifically for frustrated systems. We emphasize that its variational nature implies that the accuracy can be systematically improved by enlarging the number of states kept in the density matrix defined perpendicular to the chains (m_{s2}). This point is not a trivial one; it demands an accurate projection of the transverse Hamiltonian in an accurate representation of the Hilbert space of the chains. The systematic comparison with exact diagonalization (ED) results in two- and three-legged ladders presented here shows that in Q1D systems excellent results can be obtained with modest values for m_{s2} .

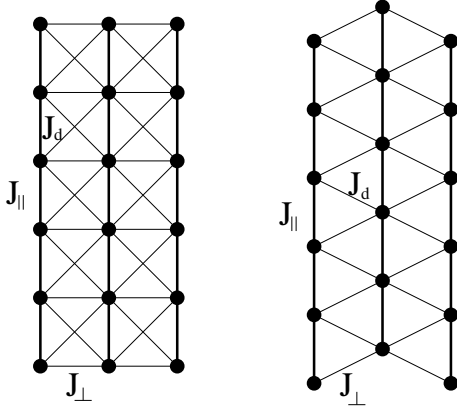


FIG. 1: The two lattice geometries studied in the text. On the left, chains coupled with perpendicular J_\perp and diagonal coupling J_d . On the right the chains are arranged on a triangular lattice.

The rest of the paper is organized as follows. The different models studied in this paper are presented in section II. Then we summarize the main steps of the algorithm implementation in section III. In section IV we show how to improve systematically the numerical results for several magnitudes exploiting the variational property of the method. In section V we study the accuracy as we increase different exchange couplings in the transverse Hamiltonians. In section VI we present our conclusions.

II. MODELS

To discuss the issues that we presented in the introductory section we need to compare the results obtained with two-step DMRG with exact data, that can be achieved by ED in small lattices¹². In addition, we want to evaluate the performance of the method for a very general class of transverse Hamiltonians including those that involve frustrating couplings between the chains (i.e., an exchange constant J_d along the diagonal of the square lattice). It is also important to study systems with different numbers of legs because they behave in a very different way as they approach the thermodynamic limit¹³.

The natural choice as test models are then the Heisenberg two- or three-legged ladders in the strong coupling limit:

$$\begin{aligned}
 H &= H_\parallel + H_\perp + H_d \\
 H_\parallel &= J_\parallel \sum_{j,l} \mathbf{S}_{j,l} \mathbf{S}_{j+1,l} \\
 H_\perp &= J_\perp \sum_{j,l} \mathbf{S}_{j,l} \mathbf{S}_{j,l+1} \\
 H_d &= J_d \sum_{j,l} (\mathbf{S}_{j,l} \mathbf{S}_{j+1,l+1} + \mathbf{S}_{j+1,l} \mathbf{S}_{j,l+1})
 \end{aligned}$$

where $J_\parallel > J_\perp, J_d$. $\mathbf{S}_{j,l}$ represents the spin operator in

the site j of chain l with the indices running $i = j \dots L_x$ and $l = 2, 3$. We impose open boundary conditions in the two directions. The coupling J_d connects spin operators along the diagonal and introduces frustration in the model.

Another frustrated model of great interest is the system of weakly coupled chains arranged in an anisotropic triangular lattice which can be written in the form

$$H = H_\parallel + H_\perp + H'_\perp \quad (1)$$

where the new term H'_\perp is:

$$H'_\perp = J_d \sum_{j,l} \mathbf{S}_{j,l} \mathbf{S}_{j+1,l+1} \quad (2)$$

Note that the model in the square lattice with diagonal couplings (1) reduces to the model defined in the triangular lattice 1 when one of the two diagonal couplings is set to zero.

III. METHOD AND DATA ANALYSIS

A detailed description of the two-step DMRG method, which we will refer for short 2S-DMRG, has been given in Refs. 2 and 3.

The exact spectrum of a single AF chain is known from the Bethe ansatz, but eigenfunctions are not easily accessible. Thus, the density-matrix renormalization group (DMRG) method^{10,11} will be used to compute an approximate spectrum $\epsilon_n, |\phi_n\rangle$ of a single chain. A preliminary account of this approach² as well as an extensive comparison with the Quantum Monte Carlo method was presented elsewhere³. By expressing the Hamiltonian on the basis generated by the tensor product of the states of different chains one obtains, up to the second order, the effective one-dimensional Hamiltonian,

$$\begin{aligned}
 \tilde{H} \approx \sum_{[n]} E_{\parallel[n]} |\Phi_{\parallel[n]}\rangle \langle \Phi_{\parallel[n]}| + J_\perp \sum_l \tilde{\mathbf{S}}_l \tilde{\mathbf{S}}_{l+1} + \\
 J_d \sum_l \tilde{\mathbf{S}}_l \tilde{\mathbf{S}}_{l+1} + \dots \quad (3)
 \end{aligned}$$

where the composite chain-spin operators on the chain l are $\tilde{\mathbf{S}}_l = (\tilde{\mathbf{S}}_{1l}, \tilde{\mathbf{S}}_{2l}, \dots, \tilde{\mathbf{S}}_{Ll})$, L_x is the chain length. The matrix elements of the first order local spin operators are respectively

$$\tilde{\mathbf{S}}_{i,l}^{n_l, m_l} = \langle \phi_{n_l} | \mathbf{S}_{i,l} | \phi_{m_l} \rangle \quad (4)$$

We will study the following magnitudes. The ground state energy per site $E_G = E_0/L$, where $L = L_x L_y$, the gap to the first excited state in the sector of spin $S_z = 0$, Δ_0 and $S_z = 1$, Δ_1 . To monitor both gaps, that have to be equal in a spin rotational invariant Hamiltonian, is a very astringent probe of the reliability of the method. The interchain spin flip coupling

TABLE I: Ground state energy per site (E_G), gaps to the $S_z = 0$ (Δ_0) and $S_z = 1$ (Δ_1) excitations and binding energy for a 2x10 leg-ladder with $J_\perp = 0.1$, $\rho = 0.0$ as a function of the number of states kept in the parallel and perpendicular direction.

2x10		E_G	Δ_0	Δ_1	E_B
ED		-0.4273296	0.283182	0.283182	-0.0015261
m_{s1}	m_{s2}	E_0	Δ_0	Δ_1	E_B
8	8	-0.42433209	0.48038304	0.28121407	-0.00083699
8	16	-0.42443195	0.47999406	0.27884533	-0.00093685
8	32	-0.42446616	0.47825339	0.27731861	-0.00097105
16	8	-0.42676461	0.29092770	0.28842390	-0.00098189
16	16	-0.42698277	0.29235105	0.28683188	-0.00120005
16	32	-0.42707158	0.28790788	0.28491220	-0.00128885
16	48	-0.42712096	0.28737740	0.28416394	-0.00133824
16	64	-0.42712439	0.28674689	0.28360519	-0.00134167
32	8	-0.42679647	0.28862051	0.28861954	-0.00099295
32	16	-0.42703063	0.29022064	0.29021987	-0.00122710
32	32	-0.42716088	0.28579872	0.28610427	-0.00135735
32	48	-0.42724324	0.28531525	0.28552398	-0.00143972
32	64	-0.42725807	0.28391776	0.28397001	-0.00145454
32	96	-0.42729144	0.28342612	0.28342613	-0.00150668

terms (e.g. $J_\perp S_{i,l}^+ S_{i,l+1}^- + \text{h.c.}$) connects different sectors with different total chain magnetization $S_T^z = \sum_i S_i^z$ that have to be accurately and consistently described by the m_{s2} states outcoming from the block renormalization step that culminates the one-dimensional part of the algorithm. This is achieved by a careful targeting of states in sectors with increasing chain magnetization S_T^z . We also computed the binding energy of the chains $E_B = (E_0(J_\perp, J_d) - E_0(J_\perp = 0, J_d = 0))/L$ which is primarily a 'transverse' magnitude. The ED data have been obtained using the Davidson algorithm¹⁴ and imposing open boundary conditions.

IV. 2S-DMRG: A CONTROLLED APPROXIMATION

The main purpose of this section is to compare the efficiency of the algorithm in frustrated and unfrustrated systems. Here we keep all the exchange couplings in the model constant and we show how the precision of the method improves systematically as we increase the number of states of the density matrix in the direction parallel (m_{s1}) and perpendicular to the chains (m_{s2}). The parallel coupling $J_\parallel = 1.0$ as the reference scale and we will keep it fixed as the reference energy scale in the problem. We present an exhaustive comparison of the 2x10 and the 3x6 ladders taking a common value of the perpendicular exchange coupling $J_\perp = 0.1$. To study the role of frustration we take two values of $J_d = \rho J_\perp$ corresponding with

TABLE II: Same magnitudes that in table I in the 2x10 frustrated ladder with $J_\perp = 0.1$ $\rho = 0.5$

2x10		E_G	Δ_0	Δ_1	E_B
ED		-0.42593175	0.319339	0.319339	-0.00012825
m_{s1}	m_{s2}	E_0	Δ_0	Δ_1	E_B
8	8	-0.42352572	0.49158956	0.31988540	-0.00003061
8	16	-0.42353999	0.49158613	0.31989184	-0.00004488
8	32	-0.42354330	0.49138272	0.31979321	-0.00004819
16	8	-0.42581768	0.32153617	0.31961081	-0.00003496
16	16	-0.42584056	0.32175918	0.31979066	-0.00005784
16	32	-0.42587346	0.32188676	0.32002579	-0.00009073
16	48	-0.42587597	0.32147706	0.31966604	-0.00009325
16	64	-0.42587630	0.32141332	0.31957621	-0.00009357
32	8	-0.42583981	0.31970010	0.31969943	-0.00003628
32	16	-0.42586676	0.31986620	0.31986620	-0.00006323
32	32	-0.42591964	0.32024093	0.32027350	-0.00011612
32	48	-0.42592399	0.31979512	0.31995252	-0.00012046
32	64	-0.42592794	0.31952783	0.31952783	-0.00012441
32	96	-0.42593076	0.31936894	0.31933910	-0.00012724

$\rho = 0$, tables I (2x10) and III (3x6) and $\rho = 0.5$, tables II (2x10) and IV(3x6), for different number of states kept in both directions. Since the Hamiltonians are anisotropic most of the energy is stored along the chains in the J_\parallel bonds and therefore we observe larger increments in accuracy when we increase m_{s1} at fixed m_{s2} than when we increase m_{s2} at fixed m_{s1} . It is also clear from this study that in all cases the singlet-triplet gap Δ_1 is closer to the exact value obtained with ED than the gap in the $S_z^T = 0$ sector Δ_0 . This is a consequence of the variational nature of the method and it is also observed in the conventional 1D DMRG: $\Delta_1 = E_0(S = 1) - E_0(S = 0)$ involves two minimal energies in different sectors and it is computed with more precision than $\Delta_0 = E_1(S = 0) - E_0(S = 0)$. However, the difference between the two gaps vanishes as m_{s1} and m_{s2} increase. Similar dependence in m_{s1} and m_{s2} is found in the anisotropic triangular lattice.

We also observe that, both in the two- and the three-leg ladder, the accuracy is always higher in the frustrated case. Actually, the improvement is one order of magnitude in all the quantities computed, irrespective of the values of m_{s1} and m_{s2} .

V. PERFORMANCE IN FRUSTRATED LATTICES.

A. Chains coupled with perpendicular and diagonal couplings

To study this point in more detail we have computed all the magnitudes listed above as a function of $\rho = J_d/J_\perp$. the results are presented in table V for the 2x10 system

TABLE III: Energies and gap dependence on the number of states kept in the 3x6 ladder with $J_\perp = 0.1$, $\rho = 0.0$.

3x6		E_G	Δ_0	Δ_1	E_B
ED		-0.41733967	0.423312	0.423312	-0.001743481
m_{s1}	m_{s2}	E_G	Δ_0	Δ_1	E_B
4	4	-0.36497451	0.32915698	0.16977127	-0.00256288
4	8	-0.36518753	0.32932855	0.17029788	-0.00277591
4	16	-0.36521796	0.32976460	0.16657322	-0.00280634
8	4	-0.41690780	0.44817021	0.44817019	-0.00111016
8	8	-0.41692515	0.42847412	0.42847414	-0.00132896
8	16	-0.41723072	0.42941491	0.42941433	-0.00163453
8	32	-0.41733685	0.42386884	0.42386885	-0.00174066

TABLE IV: Energies and gaps as a function of the number of states kept in the 3x6 ladder with $J_\perp = 0.1$ and frustration $\rho = 0.5$.

3x6		E_G	Δ_0	Δ_1	E_B
ED		-0.41580272	0.47413	0.47413	-0.00020653
m_{s1}	m_{s2}	E_G	Δ_0	Δ_1	E_B
4	4	-0.36273211	0.31690894	0.21046881	-0.00032049
4	8	-0.36274150	0.31664021	0.21032338	-0.00032987
4	16	-0.36521796	0.32976460	0.16657322	-0.00280634
8	4	-0.41565327	0.47451007	0.47451008	-0.00005708
8	8	-0.41572257	0.47473022	0.47473022	-0.00012638
8	16	-0.41579631	0.47495257	0.47495259	-0.00020012
8	32	-0.41580249	0.47415896	0.47415897	-0.00020630

and in table VI for the 3x6 system. Both E_G and E_B are non-monotonic functions of ρ with extrema in the vicinity of $\rho = 0.6$. Actually, $E_G(\rho)$ is a function concave up and $E_B(\rho)$ is concave down. The maximum in the E_B is the remnant of the decoupling between staggered parts of the coarse-grained spin operator predicted by field theory¹⁵¹⁶ at $\rho = 0.5$. In finite open-boundary systems the 'decoupling point' takes place at higher values of ρ but still can be observed through the decrease of the binding energy of the chains³. The error in the ground state energy is reduced when ρ increases, making clear that 2S-DMRG can deal with coupling Hamiltonians running along the diagonal and even more, it can perform better with frustrated than with nonfrustrated systems. A crucial observation here is that the ground state error $\delta E_0 = (E_0 - E_0^{\text{ED}})/L$ does not increase with J_d but exhibits nearly linear correlation with the value of E_B i.e it also has a minimum at $\rho \sim 0.6$. As we are going to see, this widens remarkably the range of applicability of the method.

The error in the gap $\delta \Delta_1 = |\Delta_1 - \Delta_1^{\text{ED}}|$ follows a similar trend. However, the value of $\delta \Delta_1(\rho)$ has a minimum at a value of ρ slightly higher than the error in the ground state δE_0 . The consistency of the two gaps Δ_1, Δ_0 is very

TABLE V: Energy and gap Δ_1 as a function of the ratio $\rho = J_\perp/J_\parallel$ for the 2x10 ladder with $J_\perp = 0.1$.

2×10	ρ	E_G	Δ_1	E_B
ED	0.1	-0.4268910	0.288913	-0.0010875
2S-DMRG	0.1	-0.4268418	0.28952981	-0.00103835
ED	0.2	-0.4265297	0.295369	-0.0007262
2S-DMRG	0.2	-0.4264985	0.29583873	-0.00069499
ED	0.3	-0.4262480	0.302577	-0.0004445
2S-DMRG	0.3	-0.4262304	0.30292659	-0.00042692
ED	0.4	-0.4260482	0.310563	-0.0002447
2S-DMRG	0.4	-0.4260397	0.31081613	-0.00023620
ED	0.5	-0.4259317	0.319339	-0.0001282
2S-DMRG	0.5	-0.4259279	0.31952206	-0.00012441
ED	0.6	-0.4258999	0.325816	-0.0000964
2S-DMRG	0.6	-0.4258961	0.32594461	-0.00009263
ED	0.7	-0.4259532	0.315247	-0.0001497
2S-DMRG	0.7	-0.4259449	0.3153660	-0.00014140
ED	0.8	-0.4260921	0.305058	-0.0002886
2S-DMRG	0.8	-0.4260743	0.30519779	-0.00027075
ED	0.9	-0.4263161	0.295269	-0.0005126
2S-DMRG	0.9	-0.4262837	0.29546053	-0.00048020
ED	1.0	-0.4266246	0.285893	-0.0008211
2S-DMRG	1.0	-0.4265723	0.286168	-0.00076881

high and goes beyond that the error in the gap itself $\Delta_1 - \Delta_0 < \delta \Delta_1$ warranting that the spin rotational invariance of the system is preserved by the algorithm. The difference $\Delta_1 - \Delta_0 = 5.3 \times 10^{-5}$ at $\rho = 0.0$ reduces to 1×10^{-6} at $\rho = 0.6$ in the 2x10 ladder and from 1.2×10^{-7} at $\rho = 0.0$ to 1×10^{-8} at $\rho = 0.6$ in the 3x6 ladder.

The method, being a perturbative renormalization approach, looses some precision as we increase the perturbation. In the square lattice, the strength of the perturbation can be encoded in a single parameter of the Hamiltonian J_\perp . Therefore, we observe that the precision reduces as J_\perp increases. However, when we switch on the diagonal interaction J_d for a fixed value of J_\perp the precision *increases*. Furthermore, results in tables V and VI suggest that it is not the nominal value of the transverse couplings what limits the precision of this algorithm but the value of the binding energy, which is more directly related to the expectation value of the interchain coupling Hamiltonian. To illustrate this point we have compared values of δE_0 at $\rho = 0$ and $\rho = 0.6$ (which is nearly the value of ρ with minimal binding energy). The results are presented in table VII for the 2x10 system and in table VIII for the 3x6. The precision is at least one order of magnitude higher in the $\rho = 0.6$ for both systems.

TABLE VI: Energy and gap Δ_1 as a function of the ratio $\rho = J_\perp/J_\parallel$ for the 3x6 ladder with $J_\perp = 0.1$.

3×6	ρ	E_G	Δ_1	E_B
ED	0.1	-0.41688122	0.432623	-.00128503
2S-DMRG	0.1	-0.41687959	0.43300687	-.00128340
ED	0.2	-0.41649678	0.442359	-.00090059
2S-DMRG	0.2	-0.41649591	0.44260306	-.00089972
ED	0.3	-0.4161880	0.43300687	-.00059181
2S-DMRG	0.3	-0.41618749	0.45266032	-.00059130
ED	0.4	-0.41595617	0.463113	-.00035998
2S-DMRG	0.4	-0.41595588	0.46317943	-.00035969
ED	0.5	-0.41580272	0.474130	-.00020653
2S-DMRG	0.5	-0.41580249	0.47415897	-.00020630
ED	0.6	-0.41572872	0.485568	-.00013253
2S-DMRG	0.6	-0.41572856	0.48559530	-.00013237
ED	0.7	-0.41573539	0.484843	-.00013920
2S-DMRG	0.7	-0.41573518	0.48490468	-.00013899
ED	0.8	-0.4158235	0.471902	-.00022731
2S-DMRG	0.8	-0.41582325	0.47203771	-.00022706
ED	0.9	-0.4159940	0.459162	-.00022731
2S-DMRG	0.9	-0.41599350	0.45940760	-.00039731
ED	1.0	-0.4162475	0.446652	-.00039781
2S-DMRG	1.0	-0.41624647	0.44704608	-.00065028

TABLE VII: Error in the ground state energy and exact binding energy for the 2x10 ladder at $\rho = 0.0$ and $\rho = 0.6$ for increasing values of J_\perp .

2×10	$\rho = 0.0$		$\rho = 0.6$	
J_\perp	δE_0	E_B^{ED}	δE_0	E_B^{ED}
0.05	.0000173	-.0001815	.00000093	-.00002374
0.10	.0000715	-.0007880	.00000380	-.00009639
0.15	.0001695	-.0019401	.00000849	-.00022034
0.20	.0003229	-.0037922	.00001551	-.00039864
0.25	.0005477	-.0065235	.00002530	-.00063489
0.30	.0008634	-.0103230	.00003881	-.00093364

TABLE VIII: Error in the ground state energy and exact binding energy for the 3x6 ladder at $\rho = 0.0$ and $\rho = 0.6$ for increasing values of J_\perp .

3×6	$\rho = 0.0$		$\rho = 0.6$	
J_\perp	δE_0	E_B^{ED}	δE_0	E_B^{ED}
0.05	.00000023	-.00042351	.00000003	-.00003234
0.10	.00000282	-.00174351	.00000016	-.00013256
0.15	.00001358	-.00402195	.00000052	-.00030640
0.20	.00004299	-.00729456	.00000127	-.00056073
0.25	.00010536	-.01156190	.00000275	-.00090401
0.30	.00021701	-.01678901	.00000554	-.00134668

TABLE IX: Ground state energy E_G , gap Δ_1 and binding energy of the chains E_B at different values of J'_\perp and $J_\perp = 0.3$. The number of states kept is $m_{s1} = 8, m_{s2} = 32$

3×6	J'_\perp	E_G	Δ_1	E_B
ED	0.0	-0.43238517	0.354879	-.01678898
2S-DMRG	0.0	-0.43216816	0.36016502	-.01657197
ED	0.1	-0.42595045	0.376078	-.01035425
2S-DMRG	0.1	-0.42604272	0.37907273	-.010480822
ED	0.2	-0.42136694	0.404534	-.00577075
2S-DMRG	0.2	-0.42132679	0.40566085	-.00573060
ED	0.3	-0.41878783	0.441008	-.0031642
2S-DMRG	0.3	-0.41875861	0.44085353	-.00316242
ED	0.4	-0.41876039	0.422128	-.0031642
2S-DMRG	0.4	-0.41871723	0.42255551	-.00312104
ED	0.5	-0.42172544	0.322892	-.00612925
2S-DMRG	0.5	-0.42158277	0.32995853	-.00598658
ED	0.6	-0.42805333	0.235580	-.01245714
2S-DMRG	0.6	-0.42751008	0.25335704	-.01191389

B. Chains coupled in triangular arrangements

An alternative way to couple the chain in a frustrated geometry is the anisotropic triangular lattice (see Fig 1). An additional motivation to study this system is the neutron scattering experiment in Cs_2CuCl_4 which suggests that this geometry and values of $J'_\perp = J_\perp = 0.3$ are the essential ingredients for the model Hamiltonian. Although the maximum for binding energy in this model is about $J_d = J_\perp$, the qualitative behavior of all the magnitudes studied is the same than in the lattice with diagonal couplings. With the proposed physical realization of this model in Cs_2CuCl_4 in mind, instead of presenting another extensive comparison of numerical data, we ask ourselves whether we can achieve acceptable precision in a theoretical study of that material. Therefore we focus in a value of $J_\perp = 0.3$ and increase J_d in a 3x6 ladder. The results are presented in table IX. The point $J'_\perp = J_\perp = 0.3$ turns out to be optimal because the errors are minimum in all the quantities computed.

VI. CONCLUSIONS

We have studied frustrated spin ladders using a recently proposed numerical renormalization group method for quasi-one-dimensional systems. We have presented exhaustive comparison with exact diagonalization data, a test that any other numerical method in strongly correlated systems have had to pass. The two-step DMRG method has shown good performance in a large class of frustrated systems reaching in some cases a precision comparable with the 1D case. We find a close correlation between the binding energy of the chains and the accu-

racy in the computation of ground state energy and the gap. We have also shown that a model of weakly coupled chains in a triangular geometry for Cs_2CuCl_4 is within the range of applicability of the method.

VII. ACKNOWLEDGMENTS

We would like to thank Porscha McRobbie for a critical reading of the paper and several suggestions.

-
- ¹ S. Moukouri. cond-mat/0312011
 - ² S. Moukouri and L.G. Caron, Phys. Rev. **B 67**, 092405 (2003).
 - ³ S. Moukouri. cond-mat/0305608
 - ⁴ R. Coldea, D. A. Tennant, A. M. Tsvelik, and Z. Tylczynski Phys. Rev. Lett. **86**, 1335 (2001).
 - ⁵ H.G. Evertz, G. Lana and M. Marcu, Phys. Rev. Lett. **70**, 875 (1993).
 - ⁶ A.W. Sandvik and J. Kurkijärvi, Phys. Rev. **B 43**, 5950 (1991); A.W. Sandvik, Phys. Rev. **B 59**, 14157 (1999).
 - ⁷ E. Dagotto and A. Moreo, Phys. Rev. Lett. **63**, 2148 (1989).
 - ⁸ M.S.L. du Croo de Jongh, M.J. van Leeuwen and W. van Saarloos Phys. Rev. **B 62** 14844 (2000)
 - ⁹ L. Capriotti and S. Sorella, Phys. Rev. Lett. **84**, 3173 (2000). L. Capriotti, F. Becca, A. Parola, S. Sorella Phys. Rev. Lett. **87** 097201 (2001).
 - ¹⁰ S.R. White, Phys. Rev. Lett. **69**, 2863 (1992). Phys. Rev. **B 48**, 10 345 (1993).
 - ¹¹ 'Density-Matrix Renormalization', Ed. By I. Peschel, X. Wang, M. Kaulke and K. Hallberg, Springer (1998)
 - ¹² T. Barnes, E. Dagotto, J. Riera, E.S. Swanson, Phys. Rev. **B 47** 3196 (1993)
 - ¹³ E. Dagotto and T.M. Rice. Science **271** 618 (1996).
 - ¹⁴ E.R. Davidson, J. Comp. Phys. **17** 87 (1975)
 - ¹⁵ D. Allen, F.H.L. Essler, A.A. Nersesyan. Phys. Rev. B **61** 8871 (2000).
 - ¹⁶ A.A. Nersesyan and A.M. Tsvelik, Phys. Rev. B **67**, 024422 (2003).